=> file registry
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STRUCTURE FILE UPDATES: 20 NOV 2008 HIGHEST RN 1073589-44-2 DICTIONARY FILE UPDATES: 20 NOV 2008 HIGHEST RN 1073589-44-2

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http://www.cas.org/support/stngen/stndoc/properties.html

=> file zcaplus
FILE 'ZCAPLUS' ENTERED AT 12:03:47 ON 21 NOV 2008
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FILE COVERS 1907 - 21 Nov 2008 VOL 149 ISS 22 FILE LAST UPDATED: 20 Nov 2008 (20081120/ED)

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

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L15 1 SEA FILE=ZCAPLUS ABB=ON PLU=ON L11 AND L12 L16 2 SEA FILE=ZCAPLUS ABB=ON PLU=ON L14 OR L15

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FILE 'MEDLINE' ENTERED AT 12:03:57 ON 21 NOV 2008

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L14 2 SEA FILE=ZCAPLUS ABB=ON PLU=ON L10 AND (L11 OR L12)
L15 1 SEA FILE=ZCAPLUS ABB=ON PLU=ON L11 AND L12

L15 1 SEA FILE=ZCAPLUS ABB=ON PLU=ON L11 AND L12 L16 2 SEA FILE=ZCAPLUS ABB=ON PLU=ON L14 OR L15

L17 2 SEA L16

=> dup rem L16 L17

FILE 'ZCAPLUS' ENTERED AT 12:04:10 ON 21 NOV 2008
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PROCESSING COMPLETED FOR L16 PROCESSING COMPLETED FOR L17

L18 2 DUP REM L16 L17 (2 DUPLICATES REMOVED)

ANSWERS '1-2' FROM FILE ZCAPLUS

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L18 ANSWER 1 OF 2 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 1

ACCESSION NUMBER: 2005:429490 ZCAPLUS <u>Full-text</u>

DOCUMENT NUMBER: 142:465089

TITLE: Cyanine dyes for fluorescent labeling and detecting

biological and other materials

INVENTOR(S): West, Richard Martin; Bosworth, Nigel; Mujumdar,

Ratnakar B.

PATENT ASSIGNEE(S): Amersham Biosciences UK Limited, UK; Carnegie Mellon

University

SOURCE: PCT Int. Appl., 66 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

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PRIORITY APPLN. INFO.:
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OTHER SOURCE(S):
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$$R^{3}$$
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 R^{12}
 R^{7}
 R^{13}
 R^{14}
 R^{5}
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 R^{6}
 R^{1}
 R^{1}

Title cyanine dyes are of formula (I) in which groups R3 and R4 are attached AΒ to the Z1 ring structure and groups R5 and R6 are attached to the Z2 ring structure, and n = 1, 2 or 3; Z1 and Z2 independently represent the carbon atoms necessary to complete a one ring, or two-fused ring aromatic system; at least one of groups R1, R2, R3, R4, R5, R6 and R7 is the group -E-F where E is a single bond or a spacer group and F is a target bonding group; one or more of groups R11, R12, R13 and R14 are independently selected from the group -(CH2)k-W, where W is sulfonic acid or phosphonic acid and k is an integer from 1 to 10. The dyes may be used in fluorescence labeling applications, where the presence of one and preferably multiple water solubilizing groups attached to the 3-position of the indolinium ring reduces dye-dye interactions, and hence dye-dye quenching, particularly where multiple dye mols. are attached to components such as nucleic acids, oligonucleotides, proteins and antibodies. REFERENCE COUNT: THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS 7 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 2 OF 2 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 2004:392531 ZCAPLUS Full-text

DOCUMENT NUMBER: 140:408234

TITLE: Chiral indole intermediates and their fluorescent

cyanine dyes containing functional groups for

application to biomolecules

INVENTOR(S): Mujumdar, Ratnaker B.; West, Richard Martin

PATENT ASSIGNEE(S): Carnegie Mellon University, USA; Amersham Biosciences

UK Limited

SOURCE: PCT Int. Appl., 72 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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US 20060051758				A1					US 2005-513141						20050128				
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OTHER SOURCE(S): MARPAT 140:408234

AB This invention relates to the functionalized cyanine dyes and more particularly, to the synthesis of chiral 3-substituted 2,3'-dimethyl-3H-indole and its derivs. as intermediates for preparation of cyanine dyes, to methods of preparing these dyes and the dyes so prepared, which are suitable as fluorescent labels for use with biomols. In an example, an indolium sulfonate dye was prepared from EtI and 6-(2,3-dimethyl-5-sulfo-3-hydroindol-3-yl)hexanoic acid followed by tri-Et orthoformate.

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TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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FILE COVERS 1907 - 21 Nov 2008 VOL 149 ISS 22 FILE LAST UPDATED: 20 Nov 2008 (20081120/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L9

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851528-34-2/BI OR 851528-35-3/BI OR 851528-36-4/BI OR 851528-37

-5/BI)

L9 1 SEA FILE=ZCAPLUS ABB=ON PLU=ON L8

=> d ibib abs hitstr L9 1

L9 ANSWER 1 OF 1 ZCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:429490 ZCAPLUS Full-text

DOCUMENT NUMBER: 142:465089

TITLE: Cyanine dyes for fluorescent labeling and detecting

biological and other materials

INVENTOR(S): West, Richard Martin; Bosworth, Nigel; Mujumdar,

Ratnakar B.

PATENT ASSIGNEE(S): Amersham Biosciences UK Limited, UK; Carnegie Mellon

University

SOURCE: PCT Int. Appl., 66 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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- Title cyanine dyes are of formula (I) in which groups R3 and R4 are attached to the Z1 ring structure and groups R5 and R6 are attached to the Z2 ring structure, and n = 1, 2 or 3; Z1 and Z2 independently represent the carbon atoms necessary to complete a one ring, or two-fused ring aromatic system; at least one of groups R1, R2, R3, R4, R5, R6 and R7 is the group -E-F where E is a single bond or a spacer group and F is a target bonding group; one or more of groups R11, R12, R13 and R14 are independently selected from the group (CH2)k-W, where W is sulfonic acid or phosphonic acid and k is an integer from 1 to 10. The dyes may be used in fluorescence labeling applications, where the presence of one and preferably multiple water solubilizing groups attached to the 3-position of the indolinium ring reduces dye-dye interactions, and hence dye-dye quenching, particularly where multiple dye mols. are attached to components such as nucleic acids, oligonucleotides, proteins and antibodies.
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RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; production of cyanine dyes for fluorescent labeling and detecting biol. and other materials)

RN 851528-25-1 ZCAPLUS

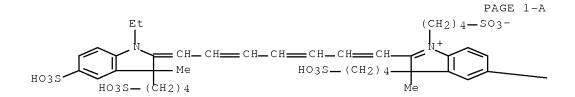
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RN 851528-28-4 ZCAPLUS

CN 3H-Indolium, 1-(5-carboxypentyl)-2-[7-[1-ethyl-1,3-dihydro-3-methyl-5-sulfo-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3,5-heptatrien-1-yl]-3-methyl-5-sulfo-3-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

RN 851528-29-5 ZCAPLUS

CN 3H-Indolium, 5-(carboxymethyl)-2-[7-[1-ethyl-1,3-dihydro-3-methyl-5-sulfo-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3,5-heptatrien-1-yl]-3-methyl-1,3-bis(4-sulfobutyl)-, inner salt (CA INDEX NAME)



PAGE 1-B

— CH2— CO2H

RN 851528-32-0 ZCAPLUS

CN 3H-Indolium, 1-(5-carboxypentyl)-2-[5-[1,3-dihydro-3-methyl-1-(phenylmethyl)-5-sulfo-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-3-methyl-5-sulfo-3-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

IT 851528-19-3P

RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

RN 851528-19-3 ZCAPLUS

CN 3H-Indolium, 1-(5-carboxypentyl)-2-[5-[1-ethyl-1,3-dihydro-3-methyl-5-sulfo-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-3-methyl-5-sulfo-3-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

IT 851528-34-2P 851528-35-3P 851528-36-4P 851528-37-5P

RL: DGN (Diagnostic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(production of cyanine dyes for fluorescent labeling and detecting biol. and other materials)

RN 851528-34-2 ZCAPLUS

CN 3H-Indolium, 2-[5-[1,3-dihydro-3-methyl-1-(phenylmethyl)-5-sulfo-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-1-[6-[(2,5-dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl]-3-methyl-5-sulfo-3-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

RN 851528-35-3 ZCAPLUS

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RN 851528-36-4 ZCAPLUS

CN 3H-Indolium, 1-[6-[(2,5-dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl]-2-[7-[1-ethyl-1,3-dihydro-3-methyl-5-sulfo-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3,5-heptatrien-1-yl]-3-methyl-5-sulfo-3-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

RN 851528-37-5 ZCAPLUS

CN 3H-Indolium, 5-[2-[(2,5-dioxo-1-pyrrolidinyl)oxy]-2-oxoethyl]-2-[7-[1-ethyl-1,3-dihydro-3-methyl-5-sulfo-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3,5-heptatrien-1-yl]-3-methyl-1,3-bis(4-sulfobutyl)-, inner salt (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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FILE 'REGISTRY' ENTERED AT 12:05:46 ON 21 NOV 2008
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Property values tagged with IC are from the ${\tt ZIC/VINITI}$ data file provided by InfoChem.

STRUCTURE FILE UPDATES: 20 NOV 2008 HIGHEST RN 1073589-44-2 DICTIONARY FILE UPDATES: 20 NOV 2008 HIGHEST RN 1073589-44-2

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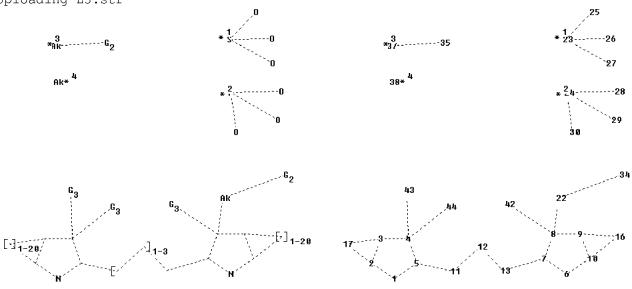
TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

Uploading L3.str



chain nodes :
22 23 24 25 26 27 28 29 30 34 35 37 38 42 43 44
ring nodes :
1 2 3 4 5 6 7 8 8 10 16 17

1 2 3 4 5 6 7 8 9 10 16 17

ring/chain nodes: 11 12 13

chain bonds :

ring/chain bonds :

5-11 11-12 12-13 ring bonds : $1-2 \quad 1-5 \quad 2-3 \quad 2-17 \quad 3-4 \quad 3-17 \quad 4-5 \quad 6-7 \quad 6-10 \quad 7-8 \quad 8-9 \quad 9-10 \quad 9-16 \quad 10-16$ exact/norm bonds : $1-2 \quad 1-5 \quad 2-3 \quad 2-17 \quad 3-4 \quad 3-17 \quad 4-5 \quad 4-43 \quad 4-44 \quad 5-11 \quad 6-7 \quad 6-10 \quad 7-8 \quad 7-13 \quad 8-9$ 8-22 8-42 9-10 9-16 10-16 11-12 12-13 22-34 23-25 23-26 23-27 24-28 24-30 24-29 35-37

G2:[*1],[*2]

G3:[*3],[*4]

Connectivity:

5:3 E exact RC ring/chain 7:3 E exact RC ring/chain 11:3 X maximum RC ring/chain 12:3 X maximum RC ring/chain 13:3 X maximum RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS 12:CLASS 13:CLASS 16:Atom 17:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS

28:CLASS 29:CLASS 30:CLASS 34:CLASS 35:CLASS 37:CLASS 38:CLASS 42:CLASS

43:CLASS 44:CLASS

Generic attributes :

22:

Type of chain : Linear Saturation : Satura : Saturated

37:

Type of chain : Linear Saturation : Saturated

=> file zcaplus FILE 'ZCAPLUS' ENTERED AT 12:05:49 ON 21 NOV 2008 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 21 Nov 2008 VOL 149 ISS 22 FILE LAST UPDATED: 20 Nov 2008 (20081120/ED)

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification. $\begin{tabular}{ll} \hline \end{tabular}$

'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L6 L3 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L5 69 SEA FILE=REGISTRY SSS FUL L3

L6 7 SEA FILE=ZCAPLUS ABB=ON PLU=ON L5

=> d ibib abs hitstr L6 1-7

L6 ANSWER 1 OF 7 ZCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2008:770729 ZCAPLUS $\underline{Full-text}$

DOCUMENT NUMBER: 149:104997

TITLE: Preparation of peptide derivatives for use as contrast

agents

INVENTOR(S): Tolleshaug, Helge; Cuthbertson, Alan; Karlsen, Hege

PATENT ASSIGNEE(S): GE Healthcare AS, Norway SOURCE: PCT Int. Appl., 53pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

GΙ

	PAT	ENT 1	NO.			KIND DATE					APPL	ICAT	DATE					
	WO	2008075968					A1 20080626			1	WO 2	 007-1		20071219				
		W: AE, AG, AL,			AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BH,	BR,	BW,	BY,	BZ,	CA,	
			CH,	CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DO,	DZ,	EC,	EE,	EG,	ES,	FΙ,
			GB,	GD,	GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,
			ΚM,	KN,	KP,	KR,	KΖ,	LA,	LC,	LK,	LR,	LS,	LT,	LU,	LY,	MA,	MD,	ME,
			MG,	MK,	MN,	MW,	MX,	MY,	MZ,	NA,	NG,	NΙ,	NO,	NΖ,	OM,	PG,	PH,	PL,
			PT,	RO,	RS,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM,	SV,	SY,	ТJ,	TM,	TN,
		TR, TT, T2		${\sf TZ}$,	UA,	UG,	US,	UZ,	VC,	VN,	ZA,	ZM,	ZW					
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			IS,	ΙΤ,	LT,	LU,	LV,	MC,	MT,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,
			ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	$\mathrm{ML}_{m{\prime}}$	MR,	NE,	SN,	TD,	TG,	BW,
			GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,
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PRIO	PRIORITY APPLN. INFO.:										NO 2006-5919					A 20061220		
]	5020	i	A 2	0071	004			
OTHER	OTHER SOURCE(S):					MARPAT 149:104997												

^{*} STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to peptide derivs. R-Sp-C-(L-P)n [the core unit C comprises amino acid residues; the linkers L may be PEG; P is a pos.-charged peptide unit; S is spacer unit, i.e., an alkyl chain or PEG; R is an imaging moiety, e.g., a radioactive or paramagnetic metal ion or a γ -emitting

radioactive halogen; p is 0 or 1; n is 1-16] which have at least one imaging moiety detectable in in vivo imaging, making the compds. useful as diagnostic contrast agents for imaging of proteoglycans, such as heparan sulfate proteoglycans. An example is peptide I which was prepared by the solid-phase method and may be chelated with a radioactive metal, preferably 99mTc.

IT 1034924-66-7P

RL: DGN (Diagnostic use); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of peptide derivs. as contrast agents)

RN 1034924-66-7 ZCAPLUS

CN INDEX NAME NOT YET ASSIGNED

PAGE 1-A

NH AcNH O

H2N—C—NH—(CH2)3—CH—C—NH

H2N—C—NH—(CH2)3—CH—C—NH—0

H2N—C—NH—(CH2)3—CH—C—NH—CH2—C—NH—CH2—C—NH—

NH

H2N—C—NH—(CH2)3—CH—C—NH—CH2—C—NH—CH2—C—NH—

H035-

PAGE 1-B

$$\begin{array}{c} - \text{NH} \\ - \text{CH} \\ - \text{NH}_{2} \end{array} \text{(CH}_{2}) \text{ 4-NH-C-CH}_{2} - \text{CH}_{2} - \text{CH}$$

PAGE 1-D

PAGE 1-E

PAGE 2-E

1034924-69-0 ITRL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of peptide derivs. as contrast agents)

RN

1034924-69-0 ZCAPLUS 3H-Indolium, 2-[5-[1-[6-[(2,5-dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl]-1,3dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-3methyl-5-sulfo-1,3-bis(4-sulfobutyl)-, inner salt, sodium salt (1:3) (CA INDEX NAME)

HO3S —
$$(CH_2)_4$$
 — $(CH_2)_4$ — $(CH_2)_4$

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 7 ZCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2007:610856 ZCAPLUS Full-text

DOCUMENT NUMBER: 147:54152

TITLE: Hydrophilic marker on the basis of diastereomeric

cyanines

INVENTOR(S): Czerney, Peter; Lehmann, Frank; Wenzel, Matthias;

Frank, Wilhelm; Schweder, Bernd

PATENT ASSIGNEE(S): Dyomics GmbH, Germany

SOURCE: Eur. Pat. Appl., 10pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PAT	CENT	NO.			KIND		DATE			APPLICATION NO.							DATE			
	EP 1792949 EP 1792949						A2 20070 A3 20080				EP	2006	5-25	20061205							
		R:		BE,												GB, SI,					
			,	HR,	MK,	YU	·	·	ŕ	•		•		•	·	·	ŕ	ŕ	·		
	DE	1020	0602	9454		A1		2007	0606		DΕ	2006	5-10	200	0602	9454	2	0060	627		
	DE	1020	0605	7345		A1		2007	0606		DE	2006	5-10	200	0605	7345	2	0061	205		
	US	2007	0128	659		A1		2007	0607		US	2006	5-56	6669	9		2	0061	205		
PRIO	RITY	APP	LN.	INFO	.:						DE	2005	5-10	200	505	8587 <i>I</i>	A 2	0051	205		
											DE	2006	5-10	200	0602	9454	A 2	0060	627		
										_											

OTHER SOURCE(S): MARPAT 147:54152

GΙ

AB The title marker for biomols. based on diastereomeric cyanines (I) and (II) (R1 and R2 = aliphatic or heteroaliph. groups, L1 - L4 = divalent linear or cyclic, optionally substituted alkylene groups, X1 = OH, SH, NH2, NHNH2, halogen, ONHS or optionally substituted groups, X2 and X3 = H, alkyl, aryl, heteroaryl, OH, SH, NH2, NHNH2, halogen, ONHS or optionally substituted groups, Y = halogen, phenoxy- or substituted arylmercapto-group) with increased solubility in water and decreased tendency to dimerization can be used in assays employing excitation light sources and luminescence detectors.

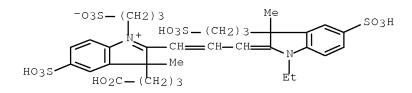
IT 939886-40-5P 939886-42-7P 939886-45-0P 939886-46-1P 939886-47-2P 939886-49-4P 939886-50-7P 939886-51-8P 939886-52-9P 939886-53-0P

RL: BUU (Biological use, unclassified); IMF (Industrial manufacture); PRP (Properties); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(enantiomer mixture; fluorescent hydrophilic marker for biomols. based on diastereomeric cyanines)

RN 939886-40-5 ZCAPLUS

CN 3H-Indolium, 3-(3-carboxypropyl)-2-[(1E)-3-[(3S,3E)-1-ethyl-1,3-dihydro-3-methyl-5-sulfo-3-(3-sulfopropyl)-2H-indol-2-ylidene]-1-propen-1-yl]-3-methyl-5-sulfo-1-(3-sulfopropyl)-, inner salt, sodium salt (1:3), (3R)-rel- (CA INDEX NAME)



●3 Na

RN 939886-42-7 ZCAPLUS

CN 3H-Indolium, 3-(3-carboxypropyl)-2-[(1E,3E)-5-[(3S,5E)-1-ethyl-1,3-dihydro-3-methyl-5-sulfo-3-(3-sulfopropyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-3-methyl-5-sulfo-1-(3-sulfopropyl)-, inner salt, sodium salt (1:3), (3R)-rel- (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

RN 939886-45-0 ZCAPLUS

CN 3H-Indolium, 3-(3-carboxypropyl)-2-[(1E,3E)-5-[(3S,5E)-1,3-dihydro-3-methyl-5-sulfo-1,3-bis(3-sulfopropyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-3-methyl-5-sulfo-1-(3-sulfopropyl)-, inner salt, sodium salt (1:4), (3R)-rel- (CA INDEX NAME)

Relative stereochemistry. Double bond geometry as shown.

RN 939886-46-1 ZCAPLUS

CN 3H-Indolium, 3-(3-carboxypropyl)-2-[(1E,3E,5E,7E)-7-[(3R)-1-ethyl-1,3-dihydro-3-methyl-5-sulfo-3-(3-sulfopropyl)-2H-indol-2-ylidene]-1,3,5-heptatrien-1-yl]-3-methyl-5-sulfo-1-(3-sulfopropyl)-, inner salt, sodium salt (1:3), (3S)-rel- (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

RN 939886-47-2 ZCAPLUS

CN 3H-Indolium, 3-(3-carboxypropyl)-2-[(1E)-2-[2-chloro-3-[(3E)-2-[(2E,3R)-1-ethyl-1,3-dihydro-3-methyl-5-sulfo-3-(3-sulfopropyl)-2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3-methyl-5-sulfo-1-(3-sulfopropyl)-, inner salt, sodium salt (1:3), (3S)-rel- (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

RN 939886-49-4 ZCAPLUS

CN 3H-Indolium, 3-(3-carboxypropyl)-2-[(1E)-3-[(3R,3E)-1-ethyl-1,3-dihydro-3-methyl-5-sulfo-3-(3-sulfopropyl)-2H-indol-2-ylidene]-1-propen-1-yl]-3-methyl-5-sulfo-1-(3-sulfopropyl)-, inner salt, sodium salt (1:3), (3R)-rel- (CA INDEX NAME)

●3 Na

RN 939886-50-7 ZCAPLUS

CN 3H-Indolium, 3-(3-carboxypropyl)-2-[(1E,3E)-5-[(3R,5E)-1-ethyl-1,3-dihydro-

3-methyl-5-sulfo-3-(3-sulfopropyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-3-methyl-5-sulfo-1-(3-sulfopropyl)-, inner salt, sodium salt (1:3), (3R)-rel- (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

RN 939886-51-8 ZCAPLUS

CN 3H-Indolium, 3-(3-carboxypropyl)-2-[(1E,3E)-5-[(3R,5E)-1,3-dihydro-3-methyl-5-sulfo-1,3-bis(3-sulfopropyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-3-methyl-5-sulfo-1-(3-sulfopropyl)-, inner salt, sodium salt (1:4), (3R)-rel- (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

RN 939886-52-9 ZCAPLUS

CN 3H-Indolium, 3-(3-carboxypropyl)-2-[(1E,3E,5E,7E)-7-[(3R)-1-ethyl-1,3-dihydro-3-methyl-5-sulfo-3-(3-sulfopropyl)-2H-indol-2-ylidene]-1,3,5-heptatrien-1-yl]-3-methyl-5-sulfo-1-(3-sulfopropyl)-, inner salt, sodium salt (1:3), (3R)-rel- (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

Na

RN 939886-53-0 ZCAPLUS

CN 3H-Indolium, 3-(3-carboxypropyl)-2-[(1E)-2-[2-chloro-3-[(3E)-2-[(2E,3S)-1-ethyl-1,3-dihydro-3-methyl-5-sulfo-3-(3-sulfopropyl)-2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3-methyl-5-sulfo-1-(3-sulfopropyl)-, inner salt, sodium salt (1:3), (3S)-rel- (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

L6 ANSWER 3 OF 7 ZCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2006:1109612 ZCAPLUS Full-text

DOCUMENT NUMBER: 145:456345

TITLE: Water-soluble fluoro-substituted cyanine dyes, as

reactive fluorescence labeling reagents, and precursor

2-methyl-3H-indole derivatives

INVENTOR(S): Cooper, Michael Edward; Gardner, Nicholas John;

Laughton, Peter Gordon

PATENT ASSIGNEE(S): Ge Healthcare UK Limited, UK SOURCE: Brit. UK Pat. Appl., 102pp.

Brit. UK Pat. Appl., 102pp CODEN: BAXXDU

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2425315	A	20061025	GB 2006-7571	20060418
AU 2006238753	A1	20061026	AU 2006-238753	20060418
CA 2605114	A1	20061026	CA 2006-2605114	20060418

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WO 2006111726
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                                                                   20060418
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PRIORITY APPLN. INFO.:
                                            GB 2005-8082
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                                            GB 2006-7571
                                                              A3 20060418
                                            WO 2006-GB1400
                                                              W 20060418
                        MARPAT 145:456345
OTHER SOURCE(S):
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GΙ

AΒ Disclosed are cyanine dyes that are useful for labeling and detecting biol. and other materials. The dyes are of formula I: in which the substituents are as defined in claim 1 and, in particular, at least one of groups R, R is -L-Mor -L-P, where L is a linking group, M is a target bonding group and P is a conjugated component, and at least one of groups R, R comprises F. The use of cyanine dyes substituted by fluorine and having addnl. substitution with three or more sulfonic acid groups for labeling biol. target mols. results in a labeled product in which there is reduced dye-dye aggregation and improved photostability, compared with cyanine dyes having no such substitutions. The dyes of the present invention are particularly useful in assays involving fluorescence detection where continual or repeated excitation is a requirement, for example in kinetic studies, or in microarray analyses where microarray slides may need to be reanalyzed over a period of days. Also disclosed are precursor 2-methyl-indolinium derivs. as defined in claim 46, as well as related cyanine dyes and 2-methyl-indolinium derivs. as defined in claims 35, 53 and 56, and 4,5,6,7-tetrafluoro-2,3-dimethyl-3H-indoles with either a 5-carboxypentyl or 4-sulfobutyl substituent in the 3-position.

IT 913198-38-6P 913198-39-7P 913198-40-0P 913198-41-1P 913198-42-2P 913198-43-3P 913198-44-4P 913198-45-5P 913198-46-6P 913198-47-7P 913198-48-8P 913198-49-9P

913198-50-2P 913198-51-3P 913198-52-4P 913198-53-5P 913198-55-7P 913198-56-8P 913198-57-9P 913198-59-1P

RL: IMF (Industrial manufacture); PRP (Properties); RGT (Reagent); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(dye; manufacture of water-soluble fluoro-substituted cyanine dyes useful

for

reactive fluorescence labeling reagents, and precursor 2-Me-3H-indole derivs.)

RN 913198-38-6 ZCAPLUS

CN 3H-Indolium, 2-[(1E,3E,5E)-5-[1-(5-carboxypentyl)-4,5,6,7-tetrafluoro-1,3-dihydro-3-methyl-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-4,5,6,7-tetrafluoro-3-methyl-1,3-bis(4-sulfobutyl)-, inner salt (CA INDEX NAME)

Double bond geometry as shown.

RN 913198-39-7 ZCAPLUS

CN 3H-Indolium, 2-[(1E,3E,5E,7E)-7-[1-(5-carboxypentyl)-4,5,6,7-tetrafluoro-1,3-dihydro-3-methyl-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3,5-heptatrien-1-yl]-4,5,6,7-tetrafluoro-3-methyl-1,3-bis(4-sulfobutyl)-, inner salt (CA INDEX NAME)

Double bond geometry as shown.

F Me
$$(CH_2)_4$$
 HO3S $(CH_2)_4$ Me F F $(CH_2)_5$ CO2H $-O_3$ S $(CH_2)_4$ F

RN 913198-40-0 ZCAPLUS

CN 3H-Indolium, 2-[(1E,3E,5E)-5-[3-(5-carboxypentyl)-1,3-dihydro-3-methyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-4,5,6,7-tetrafluoro-3-methyl-1,3-bis(4-sulfobutyl)-, inner salt (CA INDEX NAME)

RN 913198-41-1 ZCAPLUS

CN 3H-Indolium, 2-[(1E,3E,5E)-5-[1-(5-carboxypentyl)-1,3-dihydro-3-methyl-5-sulfo-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-4,5,6,7-tetrafluoro-3-methyl-1,3-bis(4-sulfobutyl)-, inner salt (CA INDEX NAME)

Double bond geometry as shown.

RN 913198-42-2 ZCAPLUS

CN 3H-Indolium, 1-(5-carboxypentyl)-2-[(1E,3E,5E)-5-[4,6-difluoro-1,3-dihydro-3-methyl-1,3-bis(4-sulfobutyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-4,5,6,7-tetrafluoro-3-methyl-3-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

Double bond geometry as shown.

RN 913198-43-3 ZCAPLUS

CN 3H-Indolium, 2-[(1E,3E,5E)-5-[1-(5-carboxypentyl)-4,6-difluoro-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-4,5,6,7-tetrafluoro-3-methyl-1,3-bis(4-sulfobutyl)-, inner salt (CA INDEX NAME)

RN 913198-44-4 ZCAPLUS

CN 3H-Indolium, 1-(5-carboxypentyl)-2-[(1E,3E,5E)-5-[1-(5-carboxypentyl)-4,6-difluoro-1,3-dihydro-3-methyl-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-4,5,6,7-tetrafluoro-3-methyl-3-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

Double bond geometry as shown.

RN 913198-45-5 ZCAPLUS

CN 3H-Indolium, 1-(5-carboxypentyl)-2-[(1E,3E,5E)-5-[1,3-dihydro-3-methyl-1,3-bis(4-sulfobutyl)-5-[(trifluoromethyl)sulfonyl]-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-4,5,6,7-tetrafluoro-3-methyl-3-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

Double bond geometry as shown.

RN 913198-46-6 ZCAPLUS

CN 3H-Indolium, 3-(5-carboxypentyl)-2-[(1E,3E,5E)-5-[4,6-difluoro-1,3-dihydro-3-methyl-1,3-bis(4-sulfobutyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-3-methyl-1-(4-sulfobutyl)-4,6-bis(trifluoromethyl)-, inner salt (CA INDEX NAME)

RN 913198-47-7 ZCAPLUS

CN 3H-Indolium, 1-(5-carboxypentyl)-2-[(1E,3E,5E)-5-[1,3-dihydro-3-methyl-1,3-bis(4-sulfobutyl)-6-(trifluoromethyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-4,5,6,7-tetrafluoro-3-methyl-3-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

Double bond geometry as shown.

RN 913198-48-8 ZCAPLUS

CN 1H-Benz[e]indolium, 2-[(1E,3E,5E)-5-[1-(5-carboxypentyl)-4,5,6,7-tetrafluoro-1,3-dihydro-3-methyl-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-4,5,6,7,8,9-hexafluoro-1,1-dimethyl-3-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

Double bond geometry as shown.

RN 913198-49-9 ZCAPLUS

CN 3H-Indolium, 2-[(1E,3E,5E)-5-[1-(5-carboxypentyl)-4,6-difluoro-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-6-fluoro-3-methyl-1,3-bis(4-sulfobutyl)-4-(trifluoromethyl)-, inner salt (CA INDEX NAME)

RN 913198-50-2 ZCAPLUS

CN 3H-Indolium, 2-[(1E,3E,5E)-5-[1-(5-carboxypentyl)-4,6-difluoro-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-4,6-difluoro-3-methyl-1,3-bis(4-sulfobutyl)-, inner salt (CA INDEX NAME)

Double bond geometry as shown.

RN 913198-51-3 ZCAPLUS

CN 3H-Indolium, 1-(5-carboxypentyl)-2-[(1E,3E,5E)-5-[1,3-dihydro-3-methyl-5-sulfo-1,3-bis(4-sulfobutyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-4,6-difluoro-3,3-dimethyl-, inner salt (CA INDEX NAME)

Double bond geometry as shown.

RN 913198-52-4 ZCAPLUS

CN 3H-Indolium, 2-[(1E,3E,5E)-5-[3-(5-carboxypentyl)-4,5,6,7-tetrafluoro-1,3-dihydro-3-methyl-1-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-4,5,6,7-tetrafluoro-3-methyl-1,3-bis(4-sulfobutyl)-, inner salt (CA INDEX NAME)

RN 913198-53-5 ZCAPLUS

CN 3H-Indolium, 2-[(1E,3E,5E)-5-[3-(5-carboxypentyl)-6-fluoro-1,3-dihydro-3-methyl-1-(4-sulfobutyl)-4-(trifluoromethyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-4,5,6,7-tetrafluoro-3-methyl-1,3-bis(4-sulfobutyl)-, inner salt (CA INDEX NAME)

Double bond geometry as shown.

RN 913198-55-7 ZCAPLUS

CN 3H-Indolium, 1-(5-carboxypentyl)-2-[(1E,3E,5E,7E)-7-[1,3-dihydro-3-methyl-1,3-bis(4-sulfobutyl)-4,6-bis(trifluoromethyl)-2H-indol-2-ylidene]-1,3,5-heptatrien-1-yl]-4,5,6,7-tetrafluoro-3-methyl-3-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

Double bond geometry as shown.

$$F_{3}$$
C F_{3} F_{3} F_{4} F_{5} $F_{$

RN 913198-56-8 ZCAPLUS

CN 3H-Indolium, 1-(5-carboxypentyl)-2-[(1E,3E,5E,7E)-7-[1,3-dihydro-3-methyl-1,3-bis(4-sulfobutyl)-5-(trifluoromethyl)-2H-indol-2-ylidene]-1,3,5-heptatrien-1-yl]-4,5,6,7-tetrafluoro-3-methyl-3-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

RN 913198-57-9 ZCAPLUS

CN 3H-Indolium, 2-[(1E,3E)-3-[1-(5-carboxypentyl)-4,5,6,7-tetrafluoro-1,3-dihydro-3-methyl-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1-propen-1-yl]-4,5,6,7-tetrafluoro-3-methyl-1,3-bis(4-sulfobutyl)-, inner salt (CA INDEX NAME)

RN 913198-58-0 ZCAPLUS

CN 3H-Indolium, 1-(5-carboxypentyl)-2-[(1E,3E)-3-[1-(5-carboxypentyl)-4,5,6,7-tetrafluoro-1,3-dihydro-3-methyl-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1-propen-1-yl]-4,5,6,7-tetrafluoro-3-methyl-3-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

RN 913198-59-1 ZCAPLUS

CN 3H-Indolium, 3-(5-carboxypentyl)-2-[(1E,3E,5E)-5-[1,3-dihydro-3-methyl-1,3-bis(4-sulfobutyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-3-methyl-5-sulfo-1-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

IT 913198-63-7P 913198-64-8P 913198-90-0P 913198-91-1P

RL: IMF (Industrial manufacture); PRP (Properties); RGT (Reagent); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(manufacture of water-soluble fluoro-substituted cyanine dyes useful for reactive fluorescence labeling reagents, and precursor 2-Me-3H-indole derivs.)

RN 913198-63-7 ZCAPLUS

CN 3H-Indolium, 2-[(1E,3E,5E)-5-[1-[6-[(2,5-dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl]-4,5,6,7-tetrafluoro-1,3-dihydro-3-methyl-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-4,5,6,7-tetrafluoro-3-methyl-1,3-bis(4-sulfobutyl)-, inner salt (CA INDEX NAME)

Double bond geometry as shown.

RN 913198-64-8 ZCAPLUS

CN 3H-Indolium, 2-[(1E,3E,5E)-5-[1-[6-[(2,5-dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl]-4,6-difluoro-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-4,5,6,7-tetrafluoro-3-methyl-1,3-bis(4-sulfobutyl)-, inner salt (CA INDEX NAME)

RN 913198-90-0 ZCAPLUS

CN 3H-Indolium, 2-[(1E,3E,5E)-5-[3-[6-[(2,5-dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl]-6-fluoro-1,3-dihydro-3-methyl-1-(4-sulfobutyl)-4-(trifluoromethyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-4,5,6,7-tetrafluoro-3-methyl-1,3-bis(4-sulfobutyl)-, inner salt (CA INDEX NAME)

Double bond geometry as shown.

RN 913198-91-1 ZCAPLUS

CN 3H-Indolium, 2-[(1E,3E,5E)-5-[3-[6-[(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)oxy]-6-oxohexyl]-6-fluoro-1,3-dihydro-3-methyl-1-(4-sulfobutyl)-4-(trifluoromethyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-4,5,6,7-tetrafluoro-3-methyl-1,3-bis(4-sulfobutyl)-, inner salt (CA INDEX NAME)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 4 OF 7 ZCAPLUS COPYRIGHT 2008 ACS on STN L6 2005:429490 ZCAPLUS Full-text ACCESSION NUMBER:

DOCUMENT NUMBER: 142:465089

TITLE: Cyanine dyes for fluorescent labeling and detecting

biological and other materials

INVENTOR(S): West, Richard Martin; Bosworth, Nigel; Mujumdar,

Ratnakar B.

Amersham Biosciences UK Limited, UK; Carnegie Mellon PATENT ASSIGNEE(S):

University

SOURCE: PCT Int. Appl., 66 pp.

CODEN: PIXXD2

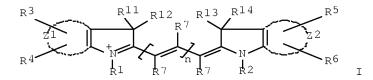
DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA	TENT	NO.			KIN	D	DATE				ICAT		DATE				
WO	2005044923			A1		20050519					20041029						
	W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	KΖ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MΖ,	NA,	NΙ,
		NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
		ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	ΑM,
		ΑZ,	BY,	KG,	KΖ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	ВG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FΙ,	FR,	GB,	GR,	HU,	ΙE,	ΙΤ,	LU,	MC,	NL,	PL,	PT,	RO,	SE,
		SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,
		SN,	TD,	ΤG													
EP	1678	258			A1		2006	0712		EP 2	004 -	7916	10		2	0041	029
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙΤ,	LI,	LU,	NL,	SE,	MC,	PT,
		ΙE,	SI,	FI,	RO,	CY,	TR,	BG,	CZ,	EE,	HU,	PL,	SK				
CN	1875	073			Α		2006	1206		CN 2	004 -	8003	2219		2	0041	029
JP	2007	5100	31		Τ		2007	0419		JP 2	006-	5374	22		2	0041	029
IN	2006	DN02	176		Α		2007	0420		IN 2	006 - 1	DN21	76		2	0060	420
US	2007	0203	343		A1		2007	0830		US 2	006-	5769	56		2	0061	127
PRIORIT	PRIORITY APPLN. INFO.:									US 2	003-	5164	28P]	P 2	0031	031
										WO 2	004-	GB45	73	Ţ	W 2	0041	029
OTHER S	OURCE	(S):			MAR:	PAT	142:	4650	89								

OTHER SOURCE(S): MARPAT 142:465089



Title cyanine dyes are of formula (I) in which groups R3 and R4 are attached AΒ to the Z1 ring structure and groups R5 and R6 are attached to the Z2 ring structure, and n = 1, 2 or 3; Z1 and Z2 independently represent the carbon atoms necessary to complete a one ring, or two-fused ring aromatic system; at least one of groups R1, R2, R3, R4, R5, R6 and R7 is the group -E-F where E is a single bond or a spacer group and F is a target bonding group; one or more of groups R11, R12, R13 and R14 are independently selected from the group -(CH2)k-W, where W is sulfonic acid or phosphonic acid and k is an integer from 1 to 10. The dyes may be used in fluorescence labeling applications, where the presence of one and preferably multiple water solubilizing groups attached to the 3-position of the indolinium ring reduces dye-dye interactions, and hence dye-dye quenching, particularly where multiple dye mols. are attached to components such as nucleic acids, oligonucleotides, proteins and antibodies. 851528-25-1P, 2-[5-[1-(5-Carboxypentyl)-3-methyl-5-sulfo-3-(4-1)]ΙT

sulfobutyl)-1,3-dihydro-2H-indol-2-ylidene]penta-1,3-dienyl]-3-methyl-1,3bis(4-sulfobutyl)-3H-indolium-5-sulfonate 851528-28-4P,
2-[7-[1-(5-Carboxypentyl)-3-methyl-5-sulfo-3-(4-sulfobutyl)-1,3-dihydro-2Hindol-2-ylidene]hepta-1,3,5-trienyl]-1-ethyl-3-methyl-3-(4-sulfobutyl)-3Hindolium-5-sulfonate 851528-29-5P 851528-32-0P,

1-Benzyl-2-[5-[1-(5-carboxypentyl)-3-methyl-5-sulfo-3-(4-sulfobutyl)-1,3-dihydro-2H-indol-2-ylidene]penta-1,3-dienyl]-3-methyl-3-(4-sulfobutyl)-3H-indolium-5-sulfonate

RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; production of cyanine dyes for fluorescent labeling and detecting biol. and other materials)

RN 851528-25-1 ZCAPLUS

CN 3H-Indolium, 1-(5-carboxypentyl)-2-[5-[1,3-dihydro-3-methyl-5-sulfo-1,3-bis(4-sulfobutyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-3-methyl-5-sulfo-3-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

RN 851528-28-4 ZCAPLUS

CN 3H-Indolium, 1-(5-carboxypentyl)-2-[7-[1-ethyl-1,3-dihydro-3-methyl-5-sulfo-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3,5-heptatrien-1-yl]-3-methyl-5-sulfo-3-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

RN 851528-29-5 ZCAPLUS

CN 3H-Indolium, 5-(carboxymethyl)-2-[7-[1-ethyl-1,3-dihydro-3-methyl-5-sulfo-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3,5-heptatrien-1-yl]-3-methyl-1,3-bis(4-sulfobutyl)-, inner salt (CA INDEX NAME)

PAGE 1-B

-- CH2- CO2H

RN 851528-32-0 ZCAPLUS

CN 3H-Indolium, 1-(5-carboxypentyl)-2-[5-[1,3-dihydro-3-methyl-1-(phenylmethyl)-5-sulfo-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-3-methyl-5-sulfo-3-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

IT 851528-19-3P

RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(production of cyanine dyes for fluorescent labeling and detecting biol.

and other materials)

RN 851528-19-3 ZCAPLUS

CN 3H-Indolium, 1-(5-carboxypentyl)-2-[5-[1-ethyl-1,3-dihydro-3-methyl-5-sulfo-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-3-methyl-5-sulfo-3-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

IT 851528-34-2P 851528-35-3P 851528-36-4P 851528-37-5P

RL: DGN (Diagnostic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(production of cyanine dyes for fluorescent labeling and detecting biol. and other materials)

RN 851528-34-2 ZCAPLUS

CN 3H-Indolium, 2-[5-[1,3-dihydro-3-methyl-1-(phenylmethyl)-5-sulfo-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-1-[6-[(2,5-dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl]-3-methyl-5-sulfo-3-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

RN 851528-35-3 ZCAPLUS

CN 3H-Indolium, 2-[5-[1,3-dihydro-3-methyl-5-sulfo-1,3-bis(4-sulfobutyl)-2H-indol-2-ylidene]-1,3-pentadien-1-yl]-1-[6-[(2,5-dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl]-3-methyl-5-sulfo-3-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

RN 851528-36-4 ZCAPLUS

CN 3H-Indolium, 1-[6-[(2,5-dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl]-2-[7-[1-ethyl-1,3-dihydro-3-methyl-5-sulfo-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3,5-heptatrien-1-yl]-3-methyl-5-sulfo-3-(4-sulfobutyl)-, inner salt (CA INDEX NAME)

RN 851528-37-5 ZCAPLUS

CN 3H-Indolium, 5-[2-[(2,5-dioxo-1-pyrrolidinyl)oxy]-2-oxoethyl]-2-[7-[1-ethyl-1,3-dihydro-3-methyl-5-sulfo-3-(4-sulfobutyl)-2H-indol-2-ylidene]-1,3,5-heptatrien-1-yl]-3-methyl-1,3-bis(4-sulfobutyl)-, inner salt (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 7 ZCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2004:392531 ZCAPLUS Full-text

DOCUMENT NUMBER: 140:408234

TITLE: Chiral indole intermediates and their fluorescent

cyanine dyes containing functional groups for

application to biomolecules

INVENTOR(S): Mujumdar, Ratnaker B.; West, Richard Martin

PATENT ASSIGNEE(S): Carnegie Mellon University, USA; Amersham Biosciences

UK Limited

SOURCE: PCT Int. Appl., 72 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA'	PATENT NO.					KIND		DATE		APPLICATION NO.				DATE			
						A2 20040513 A3 20050303		WO 2003-US14632				20030509					
WO	2004	0398	94		A3		2005	0303									
	W:	ΑE,	AG,	AL,	ΑM,	ΑT,	ΑU,	ΑZ,	ΒA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FΙ,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,
		•	•	•			SC,	•				•		•	•		
		•	•	•			VC,	•				•	·	·	·	·	·
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				A1 20040513													
	J 2003301687																
EP	1525	525265			A2 20050427			EP 2003-808367			67	20030509					
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙΤ,	LI,	LU,	NL,	SE,	MC,	PT,
		ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	HU,	SK	
JP	JP 2005536623			T	20051202			JP 2004-548262				20030509					
US	US 20060051758			A1	A1 20060309			US 2005-513141				20050128					
PRIORIT	IORITY APPLN. INFO.:								US 2	002-	3791	07P]	P 2	0020	510	
										WO 2	003-	JS14	632	Ţ	W 2	0030	509
O						m	1 40	4000	n 4								

OTHER SOURCE(S): MARPAT 140:408234

AB This invention relates to the functionalized cyanine dyes and more particularly, to the synthesis of chiral 3-substituted 2,3'-dimethyl-3H-indole and its derivs. as intermediates for preparation of cyanine dyes, to methods of preparing these dyes and the dyes so prepared, which are suitable as fluorescent labels for use with biomols. In an example, an indolium sulfonate dye was prepared from EtI and 6-(2,3-dimethyl-5-sulfo-3-hydroindol-3-yl)hexanoic acid followed by tri-Et orthoformate.

IT 688339-28-8P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; production of chiral indole intermediates and their fluorescent cyanine dyes containing functional groups for application to biomols.)

RN 688339-28-8 ZCAPLUS

CN 1H-Indole-3-hexanoic acid, 2,3-dihydro-3-methyl-2-[(2E,4E)-5-[3-methyl-5-sulfo-3-(4-sulfobutyl)-3H-indol-2-yl]-2,4-pentadien-1-ylidene]-5-sulfo-1-(4-sulfobutyl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

L6 ANSWER 6 OF 7 ZCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1994:311363 ZCAPLUS Full-text

DOCUMENT NUMBER: 120:311363 ORIGINAL REFERENCE NO.: 120:54529a

TITLE: Silver halide photographic material containing

infrared zone-absorbing filter dye

INVENTOR(S):
Harada, Tooru

PATENT ASSIGNEE(S): Fuji Photo Film Co Ltd, Japan SOURCE: Jpn. Kokai Tokkyo Koho, 20 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05313304	A	19931126	JP 1992-117583	19920511
PRIORITY APPLN. INFO.:			JP 1992-117583	19920511
OTHER SOURCE(S):	MARPAT	120:311363		

GΙ

$$\mathbb{Z}^{1}$$
 \mathbb{R}^{2}
 \mathbb{R}^{3}
 \mathbb{C}^{1}
 \mathbb{C}^{1}

AB The material contains ≥ 1 dye I (R1-6 = alkyl; R2 and/or R3, R5 and/or R6 is substituted with CO2H or SO3H; Z1, Z2 = nonmetallic atom group forming benzo and naphtho ring; R7, R9 = H, nonmetallic atom group forming 5- or 6-membered ring; R8 = H, monovalent group; X = anion; n = 1, 2) containing ≥ 4 acidic substituents. The material shows good storage stability and low level residual dye after processing.

Ι

IT 154882-02-7 154882-03-8 154882-04-9

RL: USES (Uses)

(photog. IR-filter dye)

RN 154882-02-7 ZCAPLUS

CN 3H-Indolium, 2-[7-[1,3-dihydro-3-methyl-5-sulfo-1,3-bis(4-sulfobutyl)-2H-indol-2-ylidene]-1,3,5-heptatrien-1-yl]-3-methyl-5-sulfo-1,3-bis(4-sulfobutyl)-, inner salt, potassium salt (1:5) (CA INDEX NAME)

65 K

RN 154882-03-8 ZCAPLUS

CN 3H-Indolium, 2-[2-[2-chloro-3-[2-[1,3-dihydro-3-methyl-5-sulfo-1,3-bis(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3-methyl-5-sulfo-1,3-bis(4-sulfobutyl)-, inner salt, potassium salt (1:5) (CA INDEX NAME)

●5 K

RN 154882-04-9 ZCAPLUS

CN 1H-Benz[e]indolium, 2-[2-[2-chloro-3-[2-[1,3-dihydro-1-methyl-7,9-disulfo-1,3-bis(3-sulfopropyl)-2H-benz[e]indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-1-methyl-7,9-disulfo-1,3-bis(3-sulfopropyl)-, inner salt, potassium salt (1:7) (CA INDEX NAME)

●7 K

IT 154882-01-6P

RL: PREP (Preparation)

(preparation of, photog. IR-filter dye)

RN 154882-01-6 ZCAPLUS

CN 3H-Indolium, 2-[2-[2-chloro-3-[2-[1,3-dihydro-3-methyl-1,3-bis(3-

sulfopropyl)-2H-indol-2-ylidene] = thylidene]-1-cyclohexen-1-yl] = thenyl]-3-methyl-1,3-bis(3-sulfopropyl)-, inner salt, potassium salt (1:3) (CA INDEX NAME)

●3 K

L6 ANSWER 7 OF 7 ZCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1993:157664 ZCAPLUS <u>Full-text</u>

DOCUMENT NUMBER: 118:157664

ORIGINAL REFERENCE NO.: 118:26863a,26866a

TITLE: Color proof preparation using photographic material

INVENTOR(S): Kuwajima, Shigeru; Aoki, Mario PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan SOURCE: Jpn. Kokai Tokkyo Koho, 35 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04186342	A	19920703	JP 1990-316438	19901121
PRIORITY APPLN. INFO.:			JP 1990-316438	19901121
GI				

Q1 L1 (L2 = L3)
$$\frac{1}{11}$$
 (L4 = L5) $\frac{1}{12}$ Q2 I

Q3 $\frac{1}{12}$ L6 $\frac{1}{12}$ L7 = L8) $\frac{1}{13}$ L9 = L10) $\frac{1}{14}$ Q4

AB In making half tone color proofs by color separating a color original, forming black and white half tone images following half tone conversion, exposing through the half tone images using the color separated light or its complement to form half tone color images on a color photog. material, the photog. material contains ≥1 blue sensitive emulsion layers, ≥1 green-sensitive emulsion layers, and ≥1 red-sensitive emulsion layers from unprefogged internal latent image type Ag halide emulsions, and the Ag halide emulsion layer or the hydrophilic colloid layer contains (I) [Q1, Q2 = atoms required to form a basic heterocycle; L1-5 = methine, 11, 12 = 0, 1; 11 + 12 = integer

 ≥ 1 ; ≥ 3 acid groups and present in the mol.] and(or) (II) [Q3, Q4 = atoms required to form acidic ring; L6-10 = methine group; 13, 14 = 0, 1; 13 + 14 = integer ≥ 1 ; ≥ 2 acid groups are present in the mol]. Color proofs closely resembling the original can be produced.

IT 146695-56-9

RL: USES (Uses)

(photog. material for color proofing containing)

RN 146695-56-9 ZCAPLUS

CN 3H-Benz[g]indolium, 2-[3-[1,3-dihydro-7-sulfo-1,3,3-tris(3-sulfopropyl)-2H-benz[g]indol-2-ylidene]-1-propen-1-yl]-7-sulfo-1,3,3-tris(3-sulfopropyl)-, inner salt, sodium salt (1:7) (CA INDEX NAME)

●7 Na

```
=> d his full
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     FILE 'ZCAPLUS' ENTERED AT 11:10:18 ON 21 NOV 2008
                E US2006-576956 /APPS
              1 SEA ABB=ON PLU=ON US2006-576956
L1
                                                  /AP
                D SCA
                SEL RN
     FILE 'REGISTRY' ENTERED AT 11:11:11 ON 21 NOV 2008
L2
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                D SCA
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     FILE 'REGISTRY' ENTERED AT 11:24:51 ON 21 NOV 2008
L3
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L4
              5 SEA SSS SAM L3
                D SCA
                D STAT QUE
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     FILE 'REGISTRY' ENTERED AT 11:48:13 ON 21 NOV 2008
                D STAT QUE L4
L5
             69 SEA SSS FUL L3
                SAVE TEMP CHA956STR3L/A L5
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1.6
              7 SEA ABB=ON PLU=ON L5
              1 SEA ABB=ON PLU=ON L1 AND L6
L7
                D SCA
                SEL HIT RN
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L8
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                851528-28-4/BI OR 851528-29-5/BI OR 851528-32-0/BI OR 851528-34
                -2/BI OR 851528-35-3/BI OR 851528-36-4/BI OR 851528-37-5/BI)
     FILE 'ZCAPLUS' ENTERED AT 11:53:13 ON 21 NOV 2008
L9
              1 SEA ABB=ON PLU=ON L8
                SET NOTICE OFF DISPLAY
                SET NOTICE OFF SEARCH
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L10	1823	SEA	ABB=ON	PLU=ON	WEST R?/AU
L11	17	SEA	ABB=ON	PLU=ON	BOSWORTH N?/AU
L12	29	SEA	ABB=ON	PLU=ON	MUJUMDAR R?/AU
L13	1	SEA	ABB=ON	PLU=ON	L10 AND L11 AND L12
L14	2	SEA	ABB=ON	PLU=ON	L10 AND (L11 OR L12)
L15	1	SEA	ABB=ON	PLU=ON	L11 AND L12
L16	2	SEA	ABB=ON	PLU=ON	L14 OR L15
		SET	NOTICE	LOGIN DIS	SPLAY
		SET	NOTICE	LOGIN SEA	ARCH

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FILE 'REGISTRY' ENTERED AT 12:03:42 ON 21 NOV 2008

FILE 'ZCAPLUS' ENTERED AT 12:03:47 ON 21 NOV 2008 D STAT QUE L16

FILE 'MEDLINE, EMBASE, BIOSIS, WPIX' ENTERED AT 12:03:57 ON 21 NOV 2008

D STAT QUE L17

FILE 'REGISTRY' ENTERED AT 12:04:52 ON 21 NOV 2008

FILE 'ZCAPLUS' ENTERED AT 12:04:56 ON 21 NOV 2008

D STAT QUE L9
D IBIB ABS HITSTR L9 1

FILE 'REGISTRY' ENTERED AT 12:05:46 ON 21 NOV 2008

FILE 'ZCAPLUS' ENTERED AT 12:05:49 ON 21 NOV 2008

D STAT QUE L6

D IBIB ABS HITSTR L6 1-7

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ${\tt ZIC/VINITI}$ data file provided by InfoChem.

STRUCTURE FILE UPDATES: 20 NOV 2008 HIGHEST RN 1073589-44-2 DICTIONARY FILE UPDATES: 20 NOV 2008 HIGHEST RN 1073589-44-2

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http://www.cas.org/support/stngen/stndoc/properties.html

FILE ZCAPLUS

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FILE COVERS 1907 - 21 Nov 2008 VOL 149 ISS 22 FILE LAST UPDATED: 20 Nov 2008 (20081120/ED)

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Nov 14, 2008 (20081114/UP).

FILE MEDLINE

FILE LAST UPDATED: 19 Nov 2008 (20081119/UP). FILE COVERS 1949 TO DATE.

MEDLINE has been updated with the National Library of Medicine's revised 2008 MeSH terms. See HELP RLOAD for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

See HELP RANGE before carrying out any RANGE search.

MEDLINE Accession Numbers (ANs) for records from 1950-1977 have been converted from 8 to 10 digits. Searches using an 8 or 10 digit AN will retrieve the same record. The 10-digit ANs can be expanded, searched, and displayed in all records from 1949 to the present.

FILE EMBASE

FILE COVERS 1974 TO 21 Nov 2008 (20081121/ED)

EMBASE was reloaded on March 30, 2008.

EMBASE is now updated daily. SDI frequency remains weekly (default) and biweekly.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Beginning January 2008, Elsevier will no longer provide EMTREE codes as part of the EMTREE thesaurus in EMBASE. Please update your current-awareness alerts (SDIs) if they contain EMTREE codes.

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FILE BIOSIS
FILE COVERS 1926 TO DATE.
CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT
FROM JANUARY 1926 TO DATE.

RECORDS LAST ADDED: 19 November 2008 (20081119/ED)

BIOSIS has been augmented with 1.8 million archival records from 1926 through 1968. These records have been re-indexed to match current BIOSIS indexing.

FILE WPIX

FILE LAST UPDATED: 18 NOV 2008 <20081118/UP>
MOST RECENT UPDATE: 200874 <200874/DW>
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and 20061231/UPIC, 20070601/UPIC, 20071001/UPIC, 20071130/UPIC,
20080401/UPIC, 20080701/UPIC and 20081001/UPIC.
ECLA reclassifications to mid August and US national classification
mid September 2008 have also been loaded. Update dates 20080401,
20080701 and 20081001/UPEC and /UPNC have been assigned to these. <<</pre>

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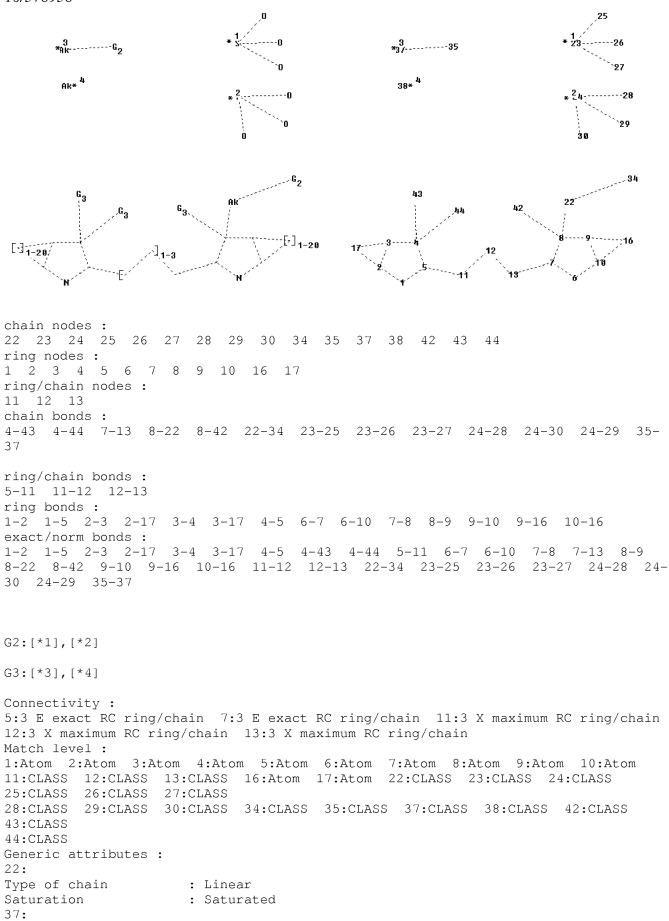
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